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Crystallographic Databases

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NIST Workshop on Crystallographic Databases

Preface

Special issues of the Journal of Research of the National Institute of Standards and Technology are devoted to papers in a particular field of measurement science. The papers herein have been written by leading experts in the field and focus on the present status and future potential of crystallographic databases. These papers, which were presented at the NIST Workshop on Crystallographic Databases, held in Gaithersburg, MD, August 1995, clearly show that crystallographic databases will have a major impact on the advancement of science and technology. Daniel B. Butrymowicz (deceased) of the materials Science and Engineering Laboratory and the NIST Publications Production Program, especially Julian Ives, deserve recognition for their dedicated efforts in producing this volume.

Vicky Lynn Karen
Alan Mighell
Special Issue Editors

Foreword

One of the most amazing facts about nature is how the fundamental particles combine into three basic building blocks—the proton, neutron and electron—under the conditions found on earth. Equally amazing is that these three particles can be aggregated into a hundred or so formations, called atoms, that form the basis of life and nature as we know it. As we aggregate atoms into molecules and compounds, the number of possible combinations becomes infinite, yet the regularity persists. This regularity of construction is marvelous, yet taken for granted.

Function follows form, and the function and properties of compounds are determined by their structure. Crystallography is the study of the structure of regular solid-state substances, and its importance is hard to overestimate. Crystallography was one of the first scientific disciplines to computerize, thereby allowing the determination of simple structures to become straightforward and of complicated structures to be possible. A natural consequence of using the computer to generate data was to use it to archive data already generated. Crystallography and neutron physics were in fact among the first areas to create numerical scientific databases. Over the last 40 years, the importance of crystallographic database work has grown enormously. Virtually all structure determinations have been archived in databases which allow easy access and complete coverage. Thousands of scientists all over the world successfully use these databases on a daily basis for a wide variety of applications.

Today, the computer revolution continues: new processors allow computations of a scale impossible just 15 years ago; database technology makes data storage and retrieval easy; and the internet makes data access trivial. How do these developments affect existing crystallographic data activities, which have evolved into a coordinated, comprehensive set of separate activities? What are the new demands that the scientific community is placing on the crystallographic data activities now that materials design from first principles is becoming a reality? Finally, what new efforts are needed to enhance the data activities, perhaps having them become more integrated? Questions such as these made it timely to organize this workshop on the crystallographic databases and to have a frank and open discussion amongst the representatives of the data activities with input from users. The reader will find in these pages not only a review of all existing crystallographic data activities, but also some answers to the questions just raised.

The NIST Standard Reference Data Program has long supported many crystallographic data efforts and is very interested in promoting discussions on issues related to the collection, evaluation, and dissemination of crystallographic data. Dr. Mary Good, Under Secretary of Technology in the U.S. Department of Commerce, joins me in thanking Vicky Lynn Karen and Alan Mighell of the NIST Crystal and Electron Diffraction Data Center for organizing the workshop and pulling together these proceedings. Opportunities for growth in terms of the nature and scope of new data activities and greater cooperation have been identified. We all look forward to further progress in meeting the need to preserve and access data on one of nature's most marvelous creations: the regularity of the structure of matter.

John Rumble, Chief
NIST Standard Reference Data Program

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Introduction

Scientific databases are becoming critical to research in the industrial and academic communities. The NIST Workshop on Crystallographic Databases was one in a series of NIST sponsored workshops each focusing on a particular type of data including, among others, crystallographic, thermodynamic, phase diagram, and mass spectral data. By bringing together top scientists involved in producing crystallographic data with users of the resulting databases, this Workshop served as a forum to examine how well the needs of the scientific community are being met and what data activities the community feels are important in the future. During the Workshop, three sessions of scientific presentations were held—(1) Formal Data Activities; (2) Scientific Uses of the Databases; and (3) Data Transfer: ensuring state of the art technology. In the first session, a representative from each of the data centers covered present activities and projected future activities of their data center. In the second session, the focus was on using crystallographic databases in analysis, in the prediction of materials properties and in the design of new chemicals, pharmaceuticals, and materials. In the third session, speakers addressed issues related to data transfer such as data exchange standards, the role of journals in the evaluation of published data, data exchange between the journals and crystallographic data centers, and computerized modes of data dissemination.

Following the presentations, a discussion session focused on Barriers to the Use of Crystallographic Data and on Partnerships for the Future. After the Workshop, the speakers submitted manuscripts which are published in this issue of the NIST Journal of Research. Following these papers are highlights of the discussion session.

As anticipated, the Workshop was attended by a diverse group who use crystallographic data in their research or are involved with this data in some other capacity, such as managers of scientific projects, journal editors, on-line system designers, instrument manufacturers, and librarians, among others. The Workshop revealed that the users of crystallographic data are being well served. The Data Centers have built evaluated databases covering all classes of compounds and they have developed theories and scientific programs for standardizing, evaluating and searching the data. Nevertheless, the topics addressed herein clearly demonstrate that the data field is in a period of dynamic transition that is being driven by many factors including a greatly increased user demand for information. Many attendees commented that the Workshop was both instructive and useful, and that it should be repeated in a few years.

The Workshop was held on August 29–30, 1995 on the campus of the National Institute of Standards and Technology (NIST) in Gaithersburg, Maryland, with the Standard Reference Data Program (SRDP) acting as host. The Workshop had no external funding, and NIST's support was fundamental to its success. We are particularly grateful to Dr. John R. Rumble, Jr., Chief of SRDP, whose support was critical for making this Workshop happen. Likewise, we appreciate the suggestions and assistance of Jean Gallagher, Sabina Crisen, and other SRDP staff members.

Many scientists contributed to the Workshop and this publication. We sincerely thank the following—David G. Watson (Cambridge Crystallographic Data Centre), Carolyn P. Brock (University of Kentucky), and Brian McMahon (International Union of Crystallography) for organizing excellent and timely sessions and for their assistance in editing the manuscripts that appear in this issue of the NIST Journal of Research; and Judith Flippen-Anderson (Naval Research Laboratory) and the attendees for a thoughtful and productive discussion session.

Vicky Lynn Karen
Alan Mighell
Special Issue Editors